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Numerical computation of eigenvalues in spectral gaps of Sturm–Liouville operators

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Abstract

We consider two different approaches for the numerical calculation of eigenvalues of a singular Sturm–Liouville problem $-y'' + Q(x)y = \lambda y$, $x \in \mathbb{R}^+$, where the potential Q is a decaying L^1 perturbation of a periodic function and the essential spectrum consequently has a band-gap structure. Both the approaches which we propose are spectrally exact: they are capable of generating approximations to eigenvalues in any gap of the essential spectrum, and do not generate any spurious eigenvalues.

We also prove (Theorem 2.4) that even the most careless of regularizations of the problem can generate at most one spurious eigenvalue in each spectral gap, a result which does not seem to have been known hitherto.

MSC: 34L16; 65L10; 65L15

Keywords: Sturm–Liouville operator; Eigenvalue problem

1. Introduction

In this paper, we consider the calculation of eigenvalues of singular Sturm–Liouville operators of the form

$$-y'' + Q(x)y = \lambda y, \quad x \in (0, \infty) \tag{1}$$

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with boundary condition

$$y(0)\cos\alpha + y'(0)\sin\alpha = 0 \tag{2}$$

for some $0 \leqslant \alpha < \pi$. The function Q is assumed to be real-valued and integrable on any finite sub-interval of $(0, \infty)$, so that $x = 0$ is a regular endpoint. Since we are interested in problems having a band-gap spectral structure, we also assume that infinity is a singular endpoint of limit-point type: in other words, the differential equation (1) has, for each λ, at most one nontrivial solution in $L^2(0, \infty)$ (see, e.g., [3]).

The limit-point assumption is necessary to ensure that the problem possesses nonempty essential spectrum, but not sufficient to guarantee the existence of essential spectrum or the existence of spectral gaps. We therefore further restrict our attention to the case where the function Q can be decomposed as

$$Q(x) = q(x) + \varepsilon r(x), \tag{3}$$

where $r \in L^1(0, \infty)$ and q is periodic with period $a > 0$:

$$q(x + a) = q(x), \quad \forall x \geqslant 0.$$

The parameter ε is a 'coupling constant' which may or may not be small.

Because of the condition $r \in L^1(0, \infty)$ it is known that the essential spectrum coincides with that of the unperturbed problem ($\varepsilon = 0$). Standard Floquet theory (see [4]) then guarantees that the essential spectrum has a band-gap structure. Generically, there are infinitely many gaps, a situation which is rather different from the PDE case according to the Bethe–Sommerfeld conjecture [6]. The spectral gaps may contain eigenvalues. The number of eigenvalues in a given gap (and even the question of whether or not this number is finite) depends not only on the behaviour of r at infinity but also on the value of the coupling constant ε: see [8] and the references therein.

We examine two different approaches to the numerical calculation of eigenvalues in gaps. In the first approach, we approximate the problem not by the classical technique of interval truncation, but rather by truncating the function r: that is, we approximate r by a function r_N having compact support contained in some half-open interval $0 \leqslant x < Na$ for some positive integer N. Standard Floquet theory allows us to identify the boundary conditions at $x = Na$ satisfied by the L^2-solution of (1) for $Q \mapsto \tilde{Q} = q + \varepsilon r_N$ when λ lies in a spectral gap. These boundary conditions are λ-dependent, and must be calculated by solving the unperturbed ($\varepsilon = 0$) differential equation over one period in order to determine the monodromy matrix. The result is a finite-interval Sturm–Liouville problem with a rather special λ-dependent boundary condition at the right endpoint $x = Na$, which we solve by shooting.

The second approach uses a result of Stolz and Weidmann [9] in order to remove the λ-dependence of the boundary condition at the right endpoint $x = Na$: one calculates the boundary condition required at $x = Na$ for some fixed $\hat{\lambda}$ in the chosen spectral gap using the same ideas as before, but one then fixes this as the λ-independent boundary condition at $x = Na$ for the truncated problem. This allows the truncated problem to be discretized to a standard λ-linear problem and solved by an appropriate method for matrix eigenproblems, which can find all the eigenvalues rather than picking them off one by one. The price which one pays for this is the following:

- Even if the original function r had compact support, it will now be necessary to allow N to tend to infinity to obtain convergence of the calculated spectra.
- The convergence of the calculated spectra as $N \to \infty$ is guaranteed to be 'exact' in the gap which contains $\hat{\lambda}$ but may generate spurious eigenvalues in other gaps.

There are not many alternatives available to the approaches presented here. For a selfadjoint operator A with a spectral gap containing a point $\mu \in \mathbb{R}$ such that $(A - \mu I)^{-1}$ exists, a variational approach applied to $(A - \mu I)^{-1}$ is possible in principle: however the calculation of the shifted resolvent requires some estimate of the L^2-solution of the differential equation for $\lambda = \mu$ and consequently offers no advantages over our algebraic technique. It would also be possible to formulate a shooting technique based on the modified Prüfer angles of Schmidt [8], but since these will satisfy a singular ODE it is likely that an approach similar to our first technique would then be required for a successful implementation.

As far as accuracy is concerned, we comment briefly on the relationship between the approaches proposed here and the approach which would perhaps come closest to being regarded as standard by numerical analysts: namely, the replacement of the differential operator by an infinite tridiagonal matrix T using the classical three point finite difference scheme:

$$T = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & 0 & 0 & \cdots \\ -1 & 2 & 1 & 0 & \cdots \\ 0 & -1 & 2 & -1 & \cdots \\ . & . & . & . & \cdots \end{pmatrix} + \operatorname{diag}(q(x_1) + \varepsilon r(x_1), q(x_2) + \varepsilon r(x_2), \ldots),$$

where for simplicity we assume that the mesh-size $h = x_{j+1} - x_j$ is constant and that the mesh fits the period of the function q exactly (that is, $h = a/M$ for some integer M). For infinite matrices of this type there is a well developed Floquet theory. It is known that there are finitely many (in fact, $O(M)$) spectral bands and that the essential spectrum ends close to some point C/h^2, where C is independent of h. Using the fact that the finite difference scheme approximates the solutions of the differential equation with order $O(h^2)$ over a finite number of periods, it may then be shown that when the perturbation r is compactly supported then the endpoints of the lower spectral bands are $O(h^2)$ accurate approximations to the endpoints of the spectral bands of the original problem. Similarly, any eigenvalues in the lower gaps will be $O(h^2)$ accurate. However the accuracy deteriorates rapidly as one proceeds to the higher parts of the spectrum, just as in the simple case of a regular problem on a compact interval, and finally breaks down totally when the essential spectrum ends at a finite point $\lambda \sim C/h^2$ for the discrete problem, but is unbounded above for the differential problem. Moreover the calculation of the spectrum of the infinite matrix T is not really any easier than what we do here for the ODE case: one must still use some sort of truncation procedure, or else exploit the discrete Floquet theory, to obtain suitable computational algorithms. For details the reader may consult the substantial literature on Jacobi matrices, starting, e.g., with the book of Teschl [10].

This paper is organized as follows. Section 2 contains an overview of the Floquet theory for the unperturbed problem. Section 3 describes the algorithms and explains why they should work. Section 4 presents the numerical results on some examples.

2. Spectral theory of (perturbed) periodic operators: a brief review

In this section, we review the Floquet theory of periodic Sturm–Liouville operators; the consequences of this theory for the perturbed case; and the spectral exactness result of Stolz and Weidmann [9] which we shall require later.

2.1. Floquet theory

For an excellent account of Floquet theory of periodic ordinary differential operators, the reader is invited to consult the book of Eastham [4, Chapter 1]. We now briefly describe the most important results required in this article.

We are interested in the 'unperturbed' equation

$$-y'' + q(x)y = \lambda y, \quad x \in (0, \infty) \tag{4}$$

subject to the boundary condition

$$y(0)\cos\alpha + y'(0)\sin\alpha = 0.$$

Here q is a periodic function with minimum period $a > 0$,

$$q(x + a) = q(x), \quad x \geqslant 0.$$

We let ϕ_1 and ϕ_2 denote the solutions of (4) subject to the initial conditions

$$\phi_1(0, \lambda) = \sin\alpha, \quad \phi_1'(0, \lambda) = \cos\alpha,$$

$$\phi_2(0, \lambda) = \cos\alpha, \quad \phi_2'(0, \lambda) = -\sin\alpha.$$

Looking for a solution of (4) which satisfies a condition of the form

$$y(x + a) = \rho y(x), \quad \rho \in \mathbb{C},$$

expressing y as a linear combination of these solutions and exploiting the periodicity of the coefficient q, it turns out that ρ must be an eigenvalue of the monodromy matrix

$$M(a, \lambda) = [\Phi(0, \lambda)]^{-1}\Phi(a, \lambda), \tag{5}$$

where

$$\Phi(x, \lambda) = \begin{pmatrix} \phi_1(x, \lambda) & \phi_2(x, \lambda) \\ \phi_1'(x, \lambda) & \phi_2'(x, \lambda) \end{pmatrix}.$$

It is easy to show that the determinant of the matrix defined in (5) is always equal to 1. The trace we denote by

$$D(\lambda) = \operatorname{trace}(M(a, \lambda)), \tag{6}$$

a quantity known as the Hill Discriminant. The values of ρ are therefore the roots of the quadratic equation

$$\rho^2 - D(\lambda)\rho + 1 = 0.$$

Since the product of the roots is 1, there are three possibilities.

$|D(\lambda)| < 2$. The roots are complex conjugate pairs and lie on the unit circle. Neither is equal to ± 1.
$|D(\lambda)| > 2$. The roots are real. One is strictly greater than 1 in absolute value, the other is strictly less than 1 in absolute value.
$|D(\lambda)| = 2$. The roots are both equal to $+1$ or both equal to -1. In these cases the differential equation possesses at least one periodic or anti-periodic solution.

Notice that it is only in the second case that the differential equation possesses a solution in $L^2(\mathbb{R}^+)$, and that when such a solution exists then it is unique up to multiplication by a scalar. Let $\rho_-(\lambda)$ and $\mathbf{v}_-(\lambda)$ be the eigenvalue and eigenvector of $M(a, \lambda)$ in this case, with $|\rho_-(\lambda)| < 1$. Then the L^2-solution is given upto a scalar by

$$\begin{pmatrix} y(x, \lambda) \\ y'(x, \lambda) \end{pmatrix} = \Phi(x, \lambda)\mathbf{v}_-(\lambda). \tag{7}$$

Remark 1. The set of values of λ for which $|D(\lambda)| < 2$ is a union of intervals, called the *stability intervals*. It is known that the closure of this set forms the essential spectrum of the associated selfadjoint differential operator.

The remaining parts of the real axis consist of *spectral gaps*, which may or may not contain isolated eigenvalues.

The endpoints of the stability intervals can also be characterized as follows. The eigenvalue problem consisting of the differential equation

$$-y'' + q(x)y = \lambda y, \quad x \in (0, a), \tag{8}$$

together with the boundary conditions

$$y(a) = y(0), \quad y'(a) = y'(0),$$

is called the *periodic* eigenvalue problem on the interval $(0, a)$. It has purely discrete spectrum $(\lambda_k)_{k\in\mathbb{N}\cup\{0\}}$. Similarly, the eigenvalue problem consisting of (8) but with the boundary conditions

$$y(a) = -y(0), \quad y'(a) = -y'(0),$$

is called the *semi-periodic* eigenvalue problem: once more its spectrum is discrete, and we denote it $(\nu_k)_{k\in\mathbb{N}\cup\{0\}}$. The following is Theorem 2.3.1 of Eastham [4].

Theorem 2.1. *The eigenvalues of the periodic and semi-periodic problems interlace in the order*

$$\lambda_0 < \nu_0 \leqslant \nu_1 < \lambda_1 \leqslant \lambda_2 < \nu_2 \leqslant \nu_3 < \lambda_3 \leqslant \lambda_4 < \cdots .$$

$D(\lambda)$ increases from -2 to 2 in the intervals $[\nu_{2m+1}, \lambda_{2m+1}]$ and decreases from 2 to -2 in the intervals $[\lambda_{2m}, \nu_{2m}]$, which are the (closures of the) stability intervals. Moreover $D(\lambda) < -2$ in the intervals (ν_{2m}, ν_{2m+1}), $D(\lambda) > 2$ in the intervals $(-\infty, \lambda_0)$ and $(\lambda_{2m+1}, \lambda_{2m+2})$, which are therefore the spectral gaps.

2.2. The effect of perturbations

We now return to our original equation (1) with potential Q given by (3). Since the function r lies in $L^1(\mathbb{R}^+)$ the perturbation to the operator caused by this function may be shown to be relatively compact, and so the essential spectrum is unchanged compared to the unperturbed case:

The essential spectrum of (1) with potential given by (3) is invariant with respect to ε.

Our objective here, however, is to regard ε as fixed, not necessarily small, and to compute numerical approximations to any eigenvalues which may be present in the spectral gaps. The usual naïve approach of truncating the infinite interval to a finite one and imposing some λ-independent boundary condition will not work. While the bands of essential spectrum will be replaced by densely clustered eigenvalues, in general this approach will also introduce many spurious eigenvalues into the spectral gaps.

The new approach is the following. Firstly, we assume in addition to the condition $r \in L^1(\mathbb{R}^+)$ the condition

$$r \text{ is bounded and } r(x) \to 0 \quad \text{as } x \to +\infty. \tag{9}$$

For each fixed $N \in \mathbb{N}$ we substitute the original problem by one in which r is replaced by a compactly supported approximation,

$$r \mapsto r_N = r\chi_{[0,Na]},$$

where $\chi_{[0,Na]}$ is the characteristic function of the interval $[0, Na]$. This approximation has two effects:

- For each N the isolated eigenvalues of the problem with r replaced by r_N can be computed as the zeros of an analytic function, which itself can be computed for each fixed λ by integrating an initial value problem over the finite interval $[0, Na]$ only. See Algorithm 3.1 below for details.
- The spectra of the problems with r replaced by r_N converge exactly to the spectra of the original problem as $N \to \infty$. See Theorem 2.2 for details.

We deal with each of these matters in turn.

Theorem 2.2. *Let $\mathscr{P}$ denote the original spectral problem consisting of* (1) *with boundary condition* (2) *and potential given by* (3). *Let $\mathscr{P}_N$ denote, for each $N \in \mathbb{N}$, the problem with r replaced by $r\chi_{[0,Na]}$. Then the following are true.*

1. *The essential spectra of $\mathscr{P}$ and $\mathscr{P}_N$ are the same.*
2. *The eigenvalues of the $\mathscr{P}_N$ converge to spectral points of $\mathscr{P}$ as $N \to \infty$.*
3. *Any spectral point of $\mathscr{P}$ is a limit of spectral points of $\mathscr{P}_N$ as $N \to \infty$.*

Proof. We let L and L_N denote the operator realizations of the differential expression (1) with boundary condition (2). From the hypothesis (9) it follows that L and L_N have the same domain

$$\mathscr{D} = \{y \in L^2(\mathbb{R}^+) \mid y, y' \in AC(\mathbb{R}^+),\ (-y'' + Qy) \in L^2(\mathbb{R}^+),\ \text{and } y \text{ satisfies (2)}\}.$$

Now we observe that

$$L_N y = Ly + (r_N - r)y = Ly - r\chi_{(Na,\infty)}y,$$

which we can write as

$$L_N = L + A_N,$$

where

$$\|A_N\| \leqslant \sup_{x \geqslant Na} |r(x)| \to 0 \quad \text{as } N \to \infty,$$

by hypothesis (9). The result is then immediate from Theorem 4.10 of Kato [7, p. 291], which gives

$$\sup_{\zeta \in \sigma(L_N)} \operatorname{dist}(\zeta, \sigma(L)) \leqslant \|A_N\|, \qquad \sup_{\zeta \in \sigma(L)} \operatorname{dist}(\zeta, \sigma(L_N)) \leqslant \|A_N\|,$$

in which $\sigma(\cdot)$ denotes the spectrum. □

2.3. A result of Stolz and Weidmann

The following theorem is just one of a number of important results in [9].

Theorem 2.3. *Suppose that a Sturm–Liouville problem $\mathscr{P}$ is posed on an interval $0 \leqslant x < b$ in which $x = 0$ is a regular endpoint and $x = b \leqslant +\infty$ is a singular endpoint of limit-point type. Suppose that $\hat{\lambda}$ lies in a gap in the essential spectrum of $\mathscr{P}$ and let I be the maximal interval containing $\hat{\lambda}$ and having empty intersection with the essential spectrum of $\mathscr{P}$. Let u be the unique (up to scalar multiples) L^2-solution of the Sturm–Liouville equation when the spectral parameter has the value $\hat{\lambda}$. Then the family $\mathscr{P}_\beta$, $\beta \in (0, b)$, of regular Sturm–Liouville problems on the intervals $0 \leqslant x \leqslant \beta$ with the same boundary condition as $\mathscr{P}$ at $x = 0$ and the boundary condition*

$$y(\beta)u'(\beta) - y'(\beta)u(\beta) = 0$$

at $x = \beta$, is spectrally inclusive for $\mathscr{P}$, and spectrally exact for $\mathscr{P}$ in I. That is, for each spectral point λ of $\mathscr{P}$ there exists, for each β, a spectral point $\lambda(\beta)$ of $\mathscr{P}_\beta$ such that $\lim_{\beta \to b} \lambda(\beta) = \lambda$; and if $(\lambda(\beta))_{\beta \in (0,b)}$ is a sequence in which $\lambda(\beta)$ lies in the spectrum of $\mathscr{P}_\beta$ and $\lambda := \lim_{\beta \to b} \lambda(\beta)$ exists and lies in I, then λ is a spectral point of $\mathscr{P}$.

2.4. The number of spurious eigenvalues in a spectral gap

In this section, we use the result of Stolz and Weidmann to prove the following result, which appears to be new.

Theorem 2.4. *Suppose that interval truncation is used to solve a singular Sturm–Liouville problem having a nontrivial gap in a nontrivial essential spectrum. Then any spectrally inclusive sequence of truncated problems generates at most one spurious eigenvalue in each spectral gap.*

More precisely, in the notation of Theorem 2.3, *consider the family $\mathscr{P}_\beta$, $\beta \in (0, b)$, of regular Sturm–Liouville problems on the intervals $0 \leqslant x \leqslant \beta$ with the same boundary condition as $\mathscr{P}$* at $x = 0$ *and any boundary condition*

$$A_\beta y(\beta) - B_\beta y'(\beta) = 0$$

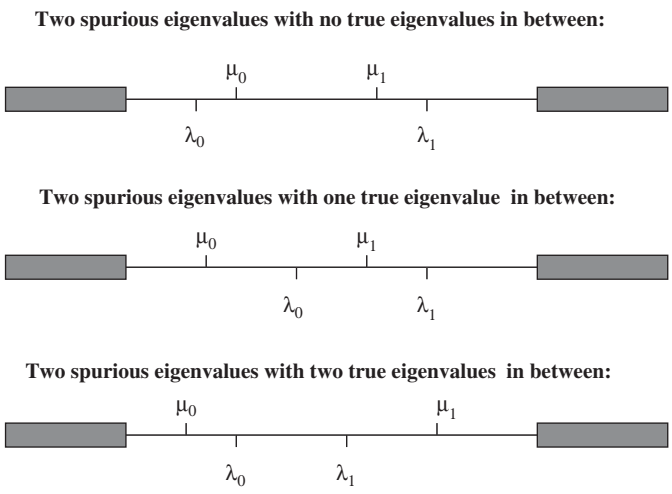

Fig. 1. True eigenvalues and spurious eigenvalues in a spectral gap: three typical cases.

at $x = \beta$, *where* $(A_\beta, B_\beta) \neq (0, 0)$. *Then in each spectral gap of* $\mathscr{P}$ *this family generates at most one spurious eigenvalue*.

Proof. The proof is by contradiction. Suppose that a sequence of truncated problems generates two spurious eigenvalues μ_0 and μ_1 in the same spectral gap: that is, there exist sequences $\mu_{0,\beta}$ and $\mu_{1,\beta}$ such that $\lim_{\beta\to\infty} \mu_{0,\beta} = \mu_0$, $\lim_{\beta\to\infty} \mu_{1,\beta} = \mu_1$, and neither μ_0 nor μ_1 is an eigenvalue of $\mathscr{P}$. There are various cases to consider.

(a) There are no eigenvalues of $\mathscr{P}$ between μ_0 and μ_1 (see Fig. 1). We use the well known eigenvalue interlacing theorem for regular problems: for each fixed β, between any two distinct eigenvalues of $\mathscr{P}_\beta$ there exists at least one eigenvalue for any other boundary condition at $x = \beta$. In particular this applies if we choose the Stolz–Weidmann boundary condition at β: let the associated eigenvalue be denoted $\lambda_\beta^{\mathrm{SW}}$, so that

$$\mu_{0,\beta} \leqslant \lambda_\beta^{\mathrm{SW}} \leqslant \mu_{1,\beta}.$$

But the Stolz–Weidmann sequence is spectrally exact, and so taking limits there must exist an eigenvalue of $\mathscr{P}$ trapped between μ_0 and μ_1. This is a contradiction.

(b) Suppose there is one eigenvalue, say λ_0, of $\mathscr{P}$ between μ_0 and μ_1 (see Fig. 1). Because the problem is assumed to have nonempty essential spectrum, it is necessarily of limit-point type, and thus according to the results of Bailey et al. [1] every sequence of truncations is spectrally inclusive regardless of the boundary conditions imposed at the truncated endpoints. In particular the sequence $\mathscr{P}_\beta$ is spectrally inclusive, and therefore possesses an eigenvalue sequence, say $\mu_{2,\beta}$, converging to λ_0. Since we have

$$\mu_{0,\beta} < \lambda_0 < \mu_{1,\beta}$$

we must have

$$\mu_{0,\beta} < \mu_{2,\beta} < \mu_{1,\beta}$$

for all sufficiently large β. Again by eigenvalue interlacing, there exist Stolz–Weidmann eigenvalues $\lambda_{0,\beta}^{\mathrm{SW}}$ in $(\mu_{0,\beta}, \mu_{2,\beta})$ and $\lambda_{1,\beta}^{\mathrm{SW}}$ in $(\mu_{2,\beta}, \mu_{1,\beta})$. Now Stolz–Weidmann eigenvalues can only converge to true eigenvalues so we must have

$$\lim_{\beta\to\infty} \lambda_{0,\beta}^{\mathrm{SW}} = \lambda_0, \quad \lim_{\beta\to\infty} \lambda_{1,\beta}^{\mathrm{SW}} = \lambda_0.$$

The fact that these two sequences have the same limit implies, by the Stolz–Weidmann spectral exactness, that λ_0 must be an eigenvalue of $\mathscr{P}$ of geometric multiplicity 2. However this is impossible for a second-order limit-point type Sturm–Liouville problem, and we again have a contradiction.

(c) The cases where there are many genuine eigenvalues trapped between μ_0 and μ_1 are treated similarly to case (b). The proof is thus complete. □

Remark 2. The previous theorem shows that one may generate at most one spurious eigenvalue at each spectral gap. Let the reader wonder whether a stronger result might be true (i.e., there are never any spurious eigenvalues) we note that using monotonicity and continuity of eigenvalues as functions of the right endpoint when a Dirichlet boundary condition is imposed there, it is not difficult to construct a sequence of truncations to generate a spurious eigenvalue at any selected point in a given spectral gap. It is less easy to see whether the construction can be made to yield, simultaneously, a spurious eigenvalue in every gap.

3. Two algorithms for numerical solution of perturbed periodic Sturm–Liouville problems

The two different algorithms considered for the numerical calculation of eigenvalues of problem (1)–(2) require the solutions of perturbed equations of the form

$$-y'' + Q(x)y = \lambda y, \quad x \in (0, Na). \tag{10}$$

Moreover, both techniques need the knowledge of a condition at $x = Na$, which can be obtained by solving the unperturbed equation

$$-y'' + q(x)y = \lambda y, \quad x \in (0, a), \tag{11}$$

determined by a suitable initial condition, as explained in Section 2.1. (The first algorithm uses the condition obtained as the basis of a shooting procedure: that is, to solve an initial value problem. For the second algorithm, the condition is to be regarded as a boundary condition associated with (10).)

The Eqs. (10) and (11) both have the form

$$-y'' + S(x)y = \lambda y, \quad x \in (c, d)$$

and can be transformed to the equivalent first order linear differential system

$$\mathbf{z}' = H(x, \lambda)\mathbf{z}, \quad x \in (c, d), \tag{12}$$

where $\mathbf{z} = (z_1, z_2)^{\mathrm{T}} = (y, y')^{\mathrm{T}}$,

$$H(x, \lambda) = \begin{pmatrix} 0 & 1 \\ S(x) - \lambda & 0 \end{pmatrix}. \tag{13}$$

Since this equation is of Hamiltonian type, it does not exhibit a preferred direction in time. It should therefore be discretised with an appropriate numerical method. A useful approach is to resort to symmetric boundary value methods (BVMs), which are also invariant under time-reversal. Introducing a partition of the interval $[c, d]$, with $x_j = c + jh$, $j = 0, 1, \ldots, n$, $h = (d-c)/n$, when applied to (12) the symmetric BVMs can be written as

$$\begin{aligned}
&\sum_{i=0}^{k} \alpha_i^{(j)} \mathbf{z}_i = h \sum_{i=0}^{k} \beta_i^{(j)} H(x_i, \lambda)\, \mathbf{z}_i, \quad j = 1, \ldots, \nu - 1,\\
&\sum_{i=0}^{k} \alpha_i \mathbf{z}_{j+i-\nu} = h \sum_{i=0}^{k} \beta_i H(x_{j+i-\nu}, \lambda) \mathbf{z}_{j+i-\nu}, \quad j = \nu, \ldots, n - \nu + 1,\\
&\sum_{i=0}^{k} \alpha_i^{(j)} \mathbf{z}_{n+i-k} = h \sum_{i=0}^{k} \beta_i^{(j)} H(x_{n+i-k}, \lambda) \mathbf{z}_{n+i-k}, \quad j = n - \nu + 2, \ldots, n
\end{aligned} \tag{14}$$

with $k = 2\nu - 1$. Further information on these methods can be found in [2]. Eq. (14) are more conveniently stated in matrix form as

$$[A \otimes I_2 - h(B \otimes \hat{H})]\mathbf{Z} = 0, \tag{15}$$

where I_2 is the identity matrix of order 2, $\otimes$ denotes the right Kronecker product,

$$A = \begin{pmatrix}
\alpha_0^{(1)} & \alpha_1^{(1)} & \cdots & \alpha_k^{(1)} & & \\
\vdots & \vdots & & \vdots & & \\
\alpha_0^{(\nu-1)} & \alpha_1^{(\nu-1)} & \cdots & \alpha_k^{(\nu-1)} & & \\
\alpha_0 & \alpha_1 & \cdots & \alpha_k & & \\
 & \ddots & \ddots & & \ddots & \\
 & & \alpha_0 & \alpha_1 & \cdots & \alpha_k \\
 & & \alpha_0^{(n-\nu+2)} & \alpha_1^{(n-\nu+2)} & \cdots & \alpha_k^{(n-\nu+2)} \\
 & & \vdots & \vdots & & \vdots \\
 & & \alpha_0^{(n)} & \alpha_1^{(n)} & \cdots & \alpha_k^{(n)}
\end{pmatrix} \in \mathbb{R}^{n\times(n+1)},$$

$$B = \begin{pmatrix}
\beta_0^{(1)} & \beta_1^{(1)} & \cdots & \beta_k^{(1)} & & \\
\vdots & \vdots & & \vdots & & \\
\beta_0^{(\nu-1)} & \beta_1^{(\nu-1)} & \cdots & \beta_k^{(\nu-1)} & & \\
\beta_0 & \beta_1 & \cdots & \beta_k & & \\
 & \ddots & \ddots & & \ddots & \\
 & & \beta_0 & \beta_1 & \cdots & \beta_k \\
 & & \beta_0^{(n-\nu+2)} & \beta_1^{(n-\nu+2)} & \cdots & \beta_k^{(n-\nu+2)} \\
 & & \vdots & \vdots & & \vdots \\
 & & \beta_0^{(n)} & \beta_1^{(n)} & \cdots & \beta_k^{(n)}
\end{pmatrix} \in \mathbb{R}^{n\times(n+1)},$$

$\hat{H} = \mathrm{diag}(H(x_0, \lambda), \ldots, H(x_n, \lambda)) \in \mathbb{R}^{(2n+2)\times(2n+2)}$ and

$$\mathbf{Z} = (\mathbf{z}_0^{\mathrm{T}}, \ldots, \mathbf{z}_n^{\mathrm{T}})^{\mathrm{T}}, \quad \mathbf{z}_j = (z_{1j}, z_{2j})^{\mathrm{T}}, \quad j = 0, 1, \ldots, n. \tag{16}$$

The numerical solution of (15) is uniquely determined by fixing appropriate initial or boundary conditions.

It follows that to obtain the condition at $x = Na$ for some fixed $\hat{\lambda}$ we have to solve two linear differential systems of type (12),

$$(\mathbf{z}^{(j)})' = \begin{pmatrix} 0 & 1 \\ q(x) - \hat{\lambda} & 0 \end{pmatrix} \mathbf{z}^{(j)}, \quad x \in (0, a), \quad j = 1, 2, \tag{17}$$

subject, respectively, to the initial conditions

$$\mathbf{z}_0^{(1)} = (\sin\alpha, \cos\alpha)^{\mathrm{T}}, \quad \mathbf{z}_0^{(2)} = (\cos\alpha, -\sin\alpha)^{\mathrm{T}}. \tag{18}$$

The numerical solutions of these two problems, denoted by

$$\mathbf{Z}^{(j)}(\hat{\lambda}) = ((\mathbf{Z}_0^{(j)}(\hat{\lambda}))^{\mathrm{T}}, \ldots, (\mathbf{Z}_n^{(j)}(\hat{\lambda}))^{\mathrm{T}})^{\mathrm{T}}, \quad j = 1, 2,$$

are uniquely determined from (15) imposing $\mathbf{Z}_0^{(j)}(\hat{\lambda}) = \mathbf{z}_0^{(j)}$, $j = 1, 2$. From them, we can define the matrix

$$\Psi(x_\ell, \hat{\lambda}) = (\mathbf{Z}_\ell^{(1)}(\hat{\lambda}), \mathbf{Z}_\ell^{(2)}(\hat{\lambda})),$$

where $x_\ell = \ell h$, $\ell = 0, 1, \ldots, n$, $h = a/n$, and an approximation of the monodromy matrix (5)

$$\hat{M}(a, \hat{\lambda}) = (\Psi(0, \hat{\lambda}))^{-1}\Psi(a, \hat{\lambda}).$$

If $|\mathrm{trace}(\hat{M}(a, \hat{\lambda}))| \leqslant 2$ we must repeat the solution of the two linear differential systems fixing another value of $\hat{\lambda}$. Otherwise, we compute the eigenvector $\mathbf{w}_-(\hat{\lambda})$ of $\hat{M}(a, \hat{\lambda})$ associated with the eigenvalue $\rho_-(\hat{\lambda})$ of modulus less than 1, since we want to select the L^2-solution of the ODE. This solution is given by (see (7))

$$\begin{pmatrix} y(x, \hat{\lambda}) \\ y'(x, \hat{\lambda}) \end{pmatrix} = \Psi(x, \hat{\lambda})\mathbf{w}_-(\hat{\lambda})$$

and hence satisfies

$$\begin{pmatrix} y(Na, \hat{\lambda}) \\ y'(Na, \hat{\lambda}) \end{pmatrix} = (\rho_-(\hat{\lambda}))^N \Psi(0, \hat{\lambda})\mathbf{w}_-(\hat{\lambda}).$$

Hence, taking $\mathbf{c}(\hat{\lambda}) = (c_1(\hat{\lambda}), c_2(\hat{\lambda}))^{\mathrm{T}} = \Psi(0, \hat{\lambda})\mathbf{w}_-(\hat{\lambda})$, we deduce the condition

$$c_2(\hat{\lambda})y(Na) - c_1(\hat{\lambda})y'(Na) = 0, \tag{19}$$

which is satisfied for each $N \in \mathbb{N}$.

3.1. Shooting technique

The solution of the $\mathscr{P}_N$ problem introduced in Theorem 2.2 is obtained by applying the parallel shooting technique coupled with an iterative method used to solve a nonlinear equation.

In particular, the procedure considered consists of introducing an initial value μ, chosen in a spectral gap, which is used to solve the two unperturbed problems given by (17) and (18) with $\hat{\lambda} = \mu$. This allows us to obtain the condition (19) used to define the differential problem

$$-y'' + Q(x)y = \mu y, \quad x \in (0, Na),$$
$$c_2(\mu)y(Na) - c_1(\mu)y'(Na) = 0.$$

This problem, written in matrix form, is

$$\mathbf{z}' = H(x, \mu)\mathbf{z}, \quad x \in (0, Na), \tag{20}$$
$$c_2(\mu)z_1(Na) - c_1(\mu)z_2(Na) = 0, \tag{21}$$

where $H(x, \mu)$ is obtained from (13) with $S(x) = Q(x)$ and $\lambda = \mu$.

To solve this sort of problem we apply the parallel shooting technique. Introducing the shooting nodes $\tau_j = ja$, $j = 0, 1, \ldots, N$, and denoting by $W_j(x) \in \mathbb{R}^{2\times 2}$, $j = 1, 2, \ldots, N$, the fundamental matrix solutions of the differential problems

$$W_j'(x) = H(x, \mu)W_j(x), \quad x \in [\tau_{j-1}, \tau_j],$$
$$W_j(\tau_j) = I_2, \quad j = 1, 2, \ldots, N, \tag{22}$$

the solution of (20) is

$$\mathbf{z}(x) = W_j(x)\mathbf{s}_j, \quad x \in [\tau_{j-1}, \tau_j], \quad j = 1, 2, \ldots, N,$$

where the vectors $\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N$, are chosen in order to ensure the continuity of $\mathbf{z}(x)$ across the interior nodes τ_j, $j = 1, 2, \ldots, N-1$, and to satisfy the condition

$$z_1(0)\cos\alpha + z_2(0)\sin\alpha = 0.$$

These requirements lead to the system

$$\begin{aligned}
&W_N(\tau_{N-1})\mathbf{s}_N = \mathbf{s}_{N-1},\\
&W_{N-1}(\tau_{N-2})\mathbf{s}_{N-1} = \mathbf{s}_{N-2},\\
&\cdots\cdots\cdots\\
&W_2(\tau_1)\mathbf{s}_2 = \mathbf{s}_1,\\
&\boldsymbol{\gamma}^{\mathrm{T}} W_1(\tau_0)\mathbf{s}_1 = 0
\end{aligned} \tag{23}$$

with $\boldsymbol{\gamma} = (\cos\alpha, \sin\alpha)^{\mathrm{T}}$, from which we have the following equation

$$\boldsymbol{\gamma}^{\mathrm{T}} W(\mu)\mathbf{s}_N = 0,$$

where $W(\mu) = W_1(\tau_0)W_2(\tau_1)\cdots W_N(\tau_{N-1})$.

The fundamental matrices $W_j(x)$, $j = 1, 2, \ldots, N$, depend on μ so that system (23) has a nontrivial solution $\mathbf{s}=(\mathbf{s}_1^{\mathrm{T}}, \mathbf{s}_2^{\mathrm{T}}, \ldots, \mathbf{s}_N^{\mathrm{T}})^{\mathrm{T}}$ if the values of μ are the eigenvalues of problem (20)–(21). In order to satisfy relation (21), we must take $\mathbf{s}_N = \mathbf{c}(\mu) = (c_1(\mu), c_2(\mu))^{\mathrm{T}}$ so that μ are approximations of the eigenvalues λ if they are solutions of equation

$$\boldsymbol{\gamma}^{\mathrm{T}} W(\mu)\mathbf{c}(\mu) = 0. \tag{24}$$

Considering that, in general, we are unable to obtain the exact solutions $W_j(x)$, $j = 1, 2, \ldots, N$, of (22), we can solve such problems applying a k-step BVM of type (14), with constant stepsize $h = a/n$, having the linear systems

$$[A \otimes I_2 - h(B \otimes \hat{H})]V^{(j)} = 0, \tag{25}$$

where $V^{(j)} = ((V_0^{(j)})^{\mathrm{T}}, \ldots, (V_n^{(j)})^{\mathrm{T}})^{\mathrm{T}}$, $V_i^{(j)} \in \mathbb{R}^{2\times 2}$, $i = 0, 1, \ldots, n$, $j = 1, 2, \ldots, N$. By fixing $V_n^{(j)} = I_2$, from (25) we can compute the matrices $V_i^{(j)}$ which are approximations of the $W_j(\tau_{j-1}+ih)$, $i = 0, 1, \ldots, n-1$, $j = 1, 2, \ldots, N$. Denoting by

$$V(\mu) = V_0^{(1)} V_0^{(2)} \cdots V_0^{(N)}$$

the discrete approximation of $W(\mu)$, instead of (24) we are reduced to solving

$$\gamma^{\mathrm{T}} V(\mu)\mathbf{c}(\mu) = 0.$$

The solutions of nonlinear problems of this type can be approximated using a classical iterative rootfinder such as, for example, bisection or the Newton method. It is important to note that at each step the matrix $V(\mu)$ and the vector $\mathbf{c}(\mu)$ must be recalculated.

3.2. Algebraic eigenvalue computation

As an alternative to the shooting technique we consider an approach similar to that introduced in [5] which consists of solving a matrix eigenproblem obtained by discretizing an appropriate boundary value problem (BVP) applying a BVM of the form (14).

We consider the differential equation

$$-y'' + Q(x)y = \lambda y, \quad x \in (0, Na) \tag{26}$$

and associated boundary conditions

$$\begin{aligned} &y(0)\cos\alpha + y'(0)\sin\alpha = 0,\\ &y(Na)c_2(\hat{\lambda}) - y'(Na)c_1(\hat{\lambda}) = 0, \end{aligned} \tag{27}$$

where the last relation is obtained from (19) with $\hat{\lambda}$ chosen in a spectral gap.

The equivalent matrix form of the BVP (26)–(27) is given by

$$\begin{aligned} &\mathbf{z}' = H(x, \lambda)\mathbf{z}, \quad x \in (0, Na),\\ &z_1(0)\cos\alpha + z_2(0)\sin\alpha = 0,\\ &z_1(Na)c_2(\hat{\lambda}) - z_2(Na)c_1(\hat{\lambda}) = 0, \end{aligned} \tag{28}$$

where $H(x, \lambda)$ is defined as in (13) with $S(x) = Q(x)$ and $\mathbf{z} = (z_1, z_2)^{\mathrm{T}} = (y, y')^{\mathrm{T}}$.

Introducing the vectors

$$\mathbf{a}_1 = (\cos\alpha, 0, \ldots, 0), \quad \mathbf{a}_2 = (\sin\alpha, 0, \ldots, 0),$$

$$\mathbf{b}_1 = (0, \ldots, 0, c_2(\hat{\lambda})), \quad \mathbf{b}_2 = (0, \ldots, 0, -c_1(\hat{\lambda}))$$

and discretizing (28), on a uniform mesh of stepsize h, by a BVM (see (14)), we obtain the matrix eigenproblem

$$E\tilde{\mathbf{Z}} = \lambda F\tilde{\mathbf{Z}}, \tag{29}$$

where $\tilde{\mathbf{Z}} = (z_{10}, z_{11}, \ldots, z_{1n}, z_{20}, z_{21}, \ldots, z_{2n})^{\mathrm{T}}$ is a suitable permutation of vector $\mathbf{Z}$ given in (16),

$$E = \begin{pmatrix} \mathbf{a}_1 & \mathbf{a}_2 \\ A & -hB \\ -hB\hat{Q} & A \\ \mathbf{b}_1 & \mathbf{b}_2 \end{pmatrix}, \quad F = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ hB & 0 \\ 0 & 0 \end{pmatrix},$$

$\hat{Q} = \mathrm{diag}(Q(x_0), Q(x_1), \ldots, Q(x_n))$ and the matrices A and B defined as in (15).

Since the matrix F is singular, we compute the eigenvalues $\xi_1, \xi_2, \ldots, \xi_{2n+2}$, of the matrix $E^{-1}F$. Being $\mathrm{rank}(E^{-1}F) = r \leqslant n$, we denote by $\xi_1, \xi_2, \ldots, \xi_r$ the nonzero eigenvalues and we set $\lambda_j = \xi_j^{-1}$, $j = 1, 2, \ldots, r$. Among $\lambda_1, \lambda_2, \ldots, \lambda_r$ we only accept as approximations to the exact eigenvalues of problem (1)–(2) the values λ_j such that $|\mathrm{trace}(\hat{M}(a, \lambda_j))| > 2$, $j \in \{1, 2, \ldots, r\}$.

This procedure allows us to find a set of eigenvalues rather than picking them off one by one as happens for the shooting technique.

4. Examples and numerical results

In the following examples we have selected the BVM given by the fourth order extended trapezoidal rule (ETR) and its boundary conditions (see [2, p. 164])

$$y_1 - y_0 = \frac{h}{24}(f_3 - 5f_2 + 19f_1 + 9f_0),$$

$$y_j - y_{j-1} = \frac{h}{24}(-f_{j+1} + 13f_j + 13f_{j-1} - f_{j-2}), \quad j = 2, \ldots, n-1,$$

$$y_n - y_{n-1} = \frac{h}{24}(f_{n-3} - 5f_{n-2} + 19f_{n-1} + 9f_n).$$

Moreover, we have chosen as iterative rootfinder the classical bisection method.

Example 1. Consider the Sturm–Liouville problem

$$-y'' + \left(\sin x + \varepsilon\frac{1}{1+x^2}\right) y = \lambda y, \quad x \in (0, \infty),$$
$$y(0)\cos\alpha + y'(0)\sin\alpha = 0. \tag{30}$$

In this case the potential $Q(x)$ given by (3) is obtained by setting

$$q(x) = \sin x,$$

$$r(x) = \frac{1}{1+x^2}.$$

Then, $q(x)$ is periodic with period $a = 2\pi$ and $r \in L^1(0, \infty)$.

Table 1
Example 1: algebraic approach

	ε_1		ε_2
	−43.8171366858787	J_1	−0.387499231924235
	−18.2531342464662		−0.347157909960590
	−7.51210141458308		−0.346280834408467
	−3.1631292135262		−0.345405172358522
	−1.7858595607726		−0.344146328795517
	−0.704097351619745		−0.342214765357849
J_1	−0.499121214887075		−0.339246090993867
	−0.436939632325172	J_2	−0.334646573722436
	−0.410336986086588		−0.327376903966521
	−0.396872180232242		−0.315449166790141
	−0.390440172134591		−0.294605042588433
	−0.389398818938790		−0.254229277705261
	−0.385038032842832		−0.161262544939272
	−0.382430017478034		0.133178437983590
	−0.380816216203125		0.918411841504191
	−0.379455268838577		0.929127808588629
	0.335936534279424	J_3	0.952772949274038
J_2	0.536620364148446		0.987964694584241
	0.580834838005921		1.25336474525398
	0.591500609480355	J_4	2.32251954775974
	0.949634991713441		
J_3	1.24466406161563		
	1.29192807845892		
J_4	2.32100272833313		

The first four gaps in the essential spectrum of this problem are the following:

$$J_1 = (-\infty, -0.3784892209), \quad J_2 = (-0.3476691249, 0.5947999710),$$

$$J_3 = (0.9180581788, 1.2931662851), \quad J_4 = (2.2851569481, 2.3425806286).$$

To obtain some numerical results we solve (30) choosing $\alpha = \pi/8$ and two different values of ε denoted by $\varepsilon_1 = -40$, $\varepsilon_2 = 60$. First of all, we have used the algebraic approach on $N = 35$ periods. We have fixed the boundary condition taking $\hat{\lambda} = 0$. The discrete problem has been solved choosing $h = 2\pi/50$. The approximate eigenvalues obtained in some spectral gaps are reported in Table 1.

Since the perturbation $\varepsilon r(x) \sim \varepsilon/x^2$ $(x \to \infty)$, Theorem 1 in [8] guarantees that an endpoint η of a spectral gap is an accumulation point of eigenvalues if

$$\frac{\varepsilon}{\varepsilon_{\text{crit}}} > 1, \quad \varepsilon_{\text{crit}} = \frac{a^2}{4|D(\lambda)|'_{|_{\lambda=\eta}}},$$

where $D(\lambda)$ is defined in (6).

Table 2
Example 1: shooting approach

N	λ_{ε_1}	λ_{ε_2}
10	0.583199585775	1.253382058825
15	0.580845364636	1.253350239771
20	0.580800129343	1.253349826409
25	0.580799631973	1.253349819501
30	0.580799627922	1.253349819373
40	0.580799627894	1.253349819371
50	0.580799627894	1.253349819371
100	0.580799627894	1.253349819371

The underlined digits are those which remain unchanged upon reduction of the stepsize h.

In fact, for $\eta = -0.3784892209$ one obtains $\varepsilon_{\text{crit}} \simeq -0.00796853$, and since $\varepsilon_1/\varepsilon_{\text{crit}} > 1$, as we can see in Table 1 this point η is an accumulation point of eigenvalues. Similar conclusions can be derived for $\eta = -0.3476691249$, being $\varepsilon_{\text{crit}} \simeq 0.00868829$ and $\varepsilon_2/\varepsilon_{\text{crit}} > 1$.

In order to compute more accurate approximations for the eigenvalues of problem (30) we use the shooting technique. In particular, we have selected in Table 1 the isolated eigenvalues $\lambda_{\varepsilon_1} = 0.580834838005921$ in the case $\varepsilon = \varepsilon_1$ and $\lambda_{\varepsilon_2} = 1.25336474525398$ for $\varepsilon = \varepsilon_2$. In Table 2 we have quoted the approximations with a constant stepsize $h = 2\pi/500$ considering some values N of periods.

Example 2. Our second example is the problem

$$\begin{aligned} &-y'' + (q(x) + \varepsilon e^{-x^2})y = \lambda y, \quad x \in (0, \infty), \\ &y(0)\theta_1 + y'(0)\theta_2 = 0, \end{aligned} \tag{31}$$

with $\theta_1 = 0.22678131377$, $\theta_2 = 0.97394570471$, and

$$q(x) = \begin{cases} 1 & 0 \leqslant x \leqslant 1, \\ 0 & 1 < x < 2. \end{cases}$$

As in the previous example, we have chosen two values of ε, i.e., $\varepsilon_3 = 1$ and $\varepsilon_4 = -1$. The problem (31) was solved by using the algebraic procedure fixing $N = 35$, $h = \frac{2}{50}$ and $\hat{\lambda} = 3$, obtaining the results reported in Table 3, where

$$\begin{aligned} &J_1 = (-\infty, 0.4808703154), \quad J_2 = (2.6453708591, 3.2818275726), \\ &J_3 = (10.3662020960, 10.3889691878), \quad J_4 = (22.6045980101, 22.8168264350), \\ &J_5 = (62.1235515268, 62.2517688274), \quad J_6 = (355.7899630282, 355.8259339049) \end{aligned}$$

are the gaps in the essential spectrum containing some eigenvalues. As one can see from the same table, in this case there are no accumulation points of eigenvalues. This happens since the perturbation $r(x) = \mathrm{e}^{-x^2}$ decays more rapidly than that considered in [8]. Moreover, we approximated some eigenvalues of problem (31) by means of the shooting approach using a discretization with stepsize $h = 10^{-2}$. In particular, in Table 4 we present the results concerning two eigenvalues λ_{ε_3} and λ_{ε_4} obtained, respectively, for $\varepsilon = \varepsilon_3$ and $\varepsilon = \varepsilon_4$.

Table 3
Example 2: algebraic approach

	ε_3		ε_4
J_1	0.480440739736803	J_1	0.175688330855064 0.480440739997243
J_2	3.15892904991076		
J_4	22.7482526804250	J_2	2.81582134947006
J_5	62.2360250184099	J_3	10.3874191453898
J_6	355.801653258160	J_4	22.6991156046360
		J_5	62.2032854370029

Table 4
Example 2: shooting approach with $h = 10^{-2}$

N	$\lambda_{\varepsilon 3}$	$\lambda_{\varepsilon 4}$
10	3.166625649204	2.784797787195
15	3.149676082052	2.798728068898
20	3.146369285339	2.801032676261
25	3.145736544349	2.801422557348
30	3.145614743591	2.801489206471
40	3.145586660909	2.801502596639
50	3.145585609812	2.801502991059
75	3.145585568933	2.801503003030
100	3.145585568922	2.801503003032

5. Conclusions

As expected, the shooting procedure was much more accurate than the algebraic technique based on the theorem of Stolz and Weidmann. This is not surprising, as the algebraic technique uses much cruder information about the behaviour of the L^2-solutions, information which, strictly speaking, is not valid outside the spectral gap for which it is calculated. One therefore ought to expect spurious eigenvalues in the 'other' gaps when using the algebraic technique. The fact that these are not manifest here is surprising and probably merits further investigation. From a numerical standpoint, what is also useful to note is that the algebraic technique, though crude, is good enough to give estimates which can rapidly be refined by the shooting method.

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